Performance Assessment Challenges and Model Abstraction

Greg Flach
Savannah River National Laboratory

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Cementitious Barriers Partnership

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PA Challenges: Long Time Scales

Disposal of long-lived radionuclides requires effective containment for 1,000 to 10,000 years or more, e.g.,

- Tank closures, saltstone
- Solid waste disposal
- D&D

However assumed performance beyond ~500 years requires explicit justification, e.g., NUREG-1573

- "Engineered barriers can . . . be assumed to have physically degraded after 500 years"
- "For timeframes longer than 500 years . . . credit . . . may be taken for the long-term provided the applicant provides suitable information and justification"

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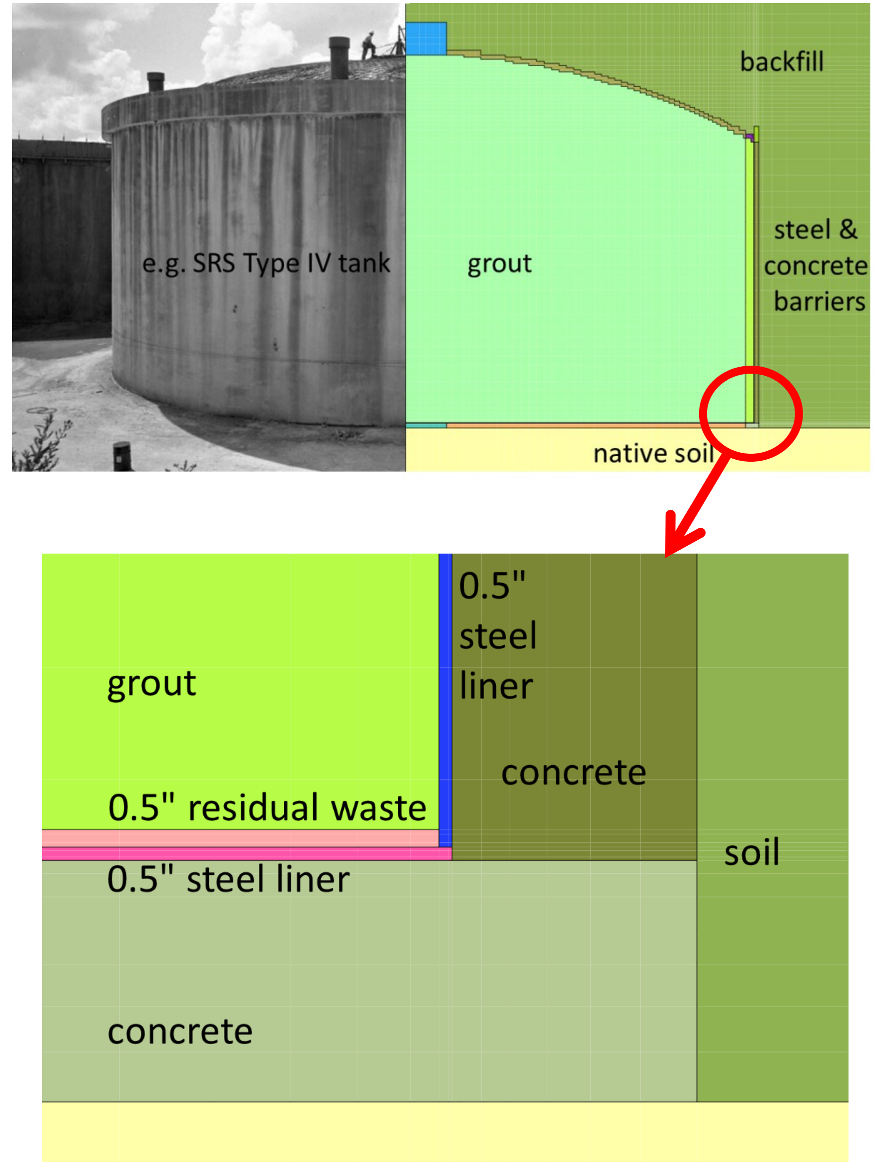
PA Challenges: Engineered Materials

Engineered barriers and waste forms introduce significant modeling challenges:

- Reactive chemistry (grout and concrete)
- Evolution of physical and chemical properties over long time periods
- Highly contrasting material properties and fine geometric features (liners and fast flow paths)



PA Challenges: Uncertainties

Significant uncertainties

- Scenarios / conceptual models
- Closure state
- Exposure conditions
- Material properties and evolution

Features
Events
Processes

Uncertainties must be reduced and/or managed

- Experimental measurement
- Field validation
- Sensitivity analysis and uncertainty quantification
- Compliance margin

⇨ **Many modeling cases**

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PA Challenges: Ambiguous Objectives

Period of Performance?

- DOE Order 435.1 → 1,000 yrs
- NRC guidance → 10,000 yrs

"Reasonable" expectation / assurance?

- Subjective criterion
- Role of behavior beyond period of performance

⇨ **More modeling cases**

PA Challenges: Computing Demands

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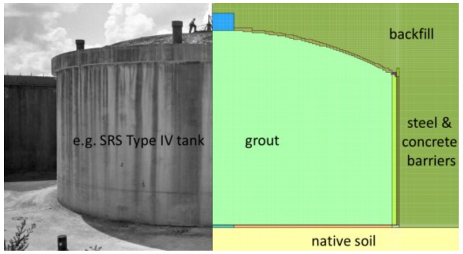


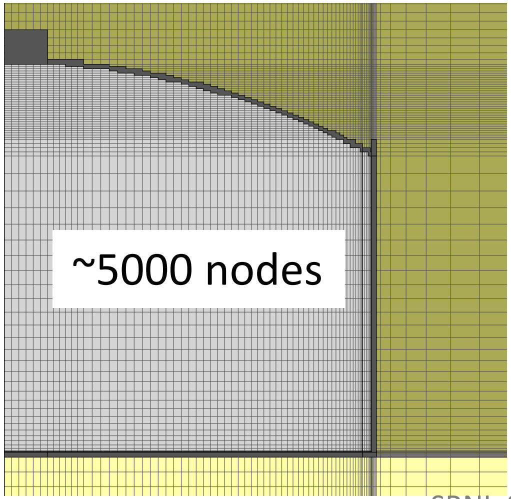
Savannah River H-Tank Farm example

Vadose zone flow

- 4000 simulations = 5 scenarios · 20 tanks/srcs · 40 flow periods

Vadose zone transport

- Base case: 3200 runs = 40 tanks/srcs · 80 species
- Alternative cases: 1000 runs = 4 cases · 25 srcs · 10 species
- Sensitivity cases: 1000 runs = 10 scenarios · 10 srcs · 10 species
- Total: 5200 simulations



Aquifer transport

- 5200 simulations

Total = 14,400 simulations

PA Challenges: Schedule Constraints

Performance Assessment

– Months to one year

Revisions

– Weeks to months

Comment response

– Days to weeks

⇨ **Modeling efficiency**

PA Challenges: Multiple Models

Higher fidelity models for separate effects/phenomena and/or very-near field

- Cementitious material degradation
- Corrosion
- Reactive chemistry

System models for deterministic and limited sensitivity analysis

- Vadose zone / near-field
- Aquifer / far-field

Abstracted system model for sensitivity analysis and uncertainty quantification

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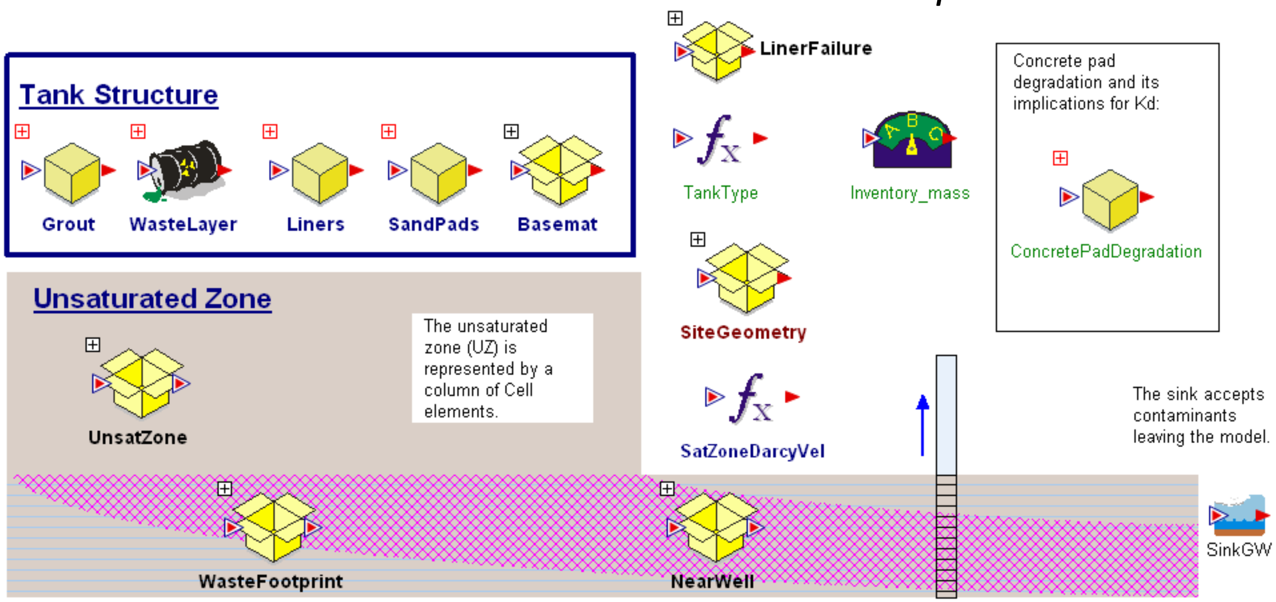
PA Challenges: Model Abstraction

Model abstraction required for efficiency

- Dimensionality: 3D → 2D → 1D
- Properties → fcn(time)
- Etc.

Savannah River H-Tank Farm example



PA Challenges: Model Integration

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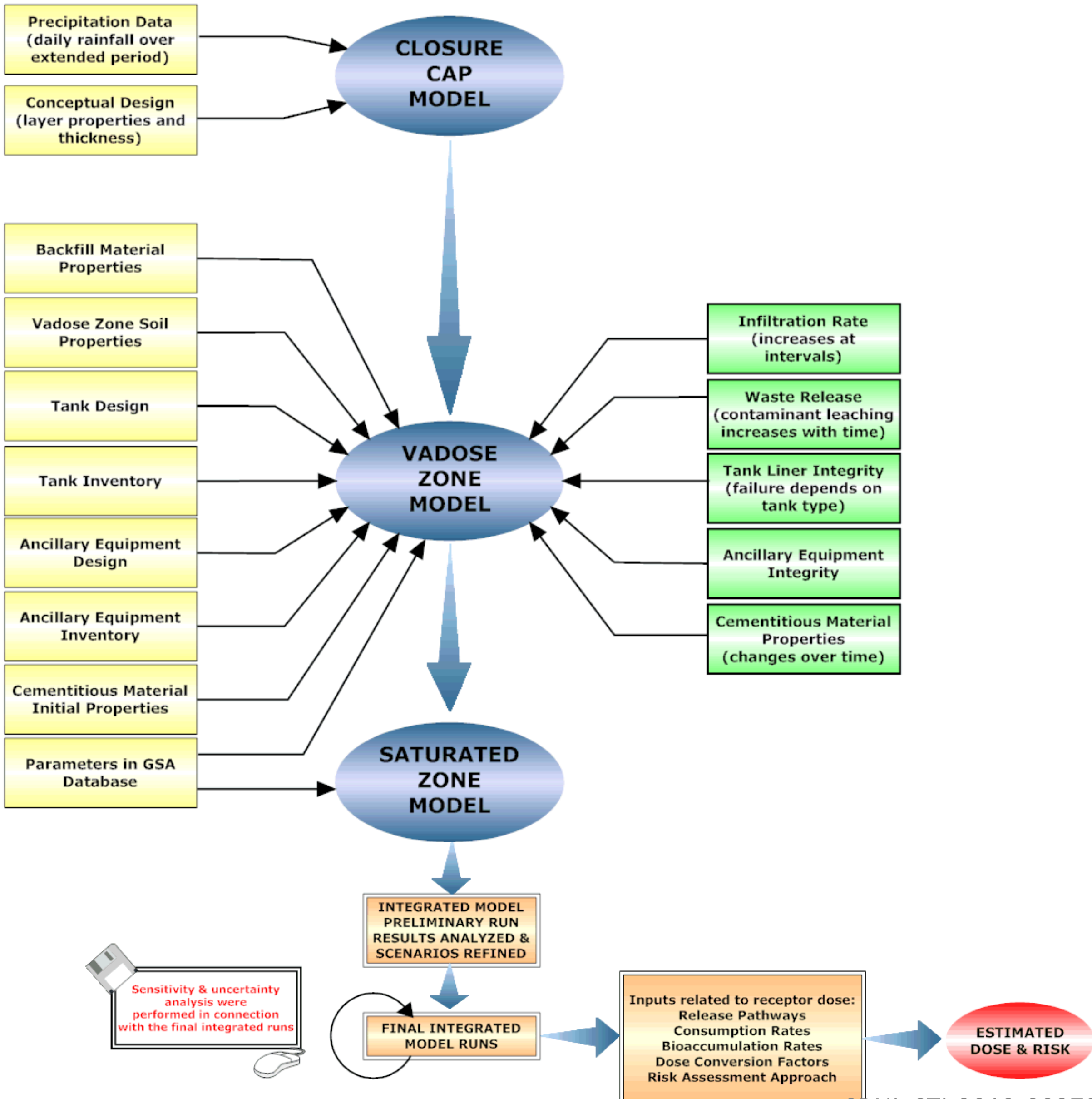
Model integration

- Phenomena
- Regions
- Varying fidelity / abstraction
- Benchmarking



CBP Products and PA Process

Higher fidelity models for simulating transport and degradation phenomena in cementitious materials

- Primary, secondary, and trace species transport
- External Sulfate Attack (~FY11)
- Carbonation (~FY12)
- Fractured materials (~FY13)

Experimental data

- Property measurements
- Validation data

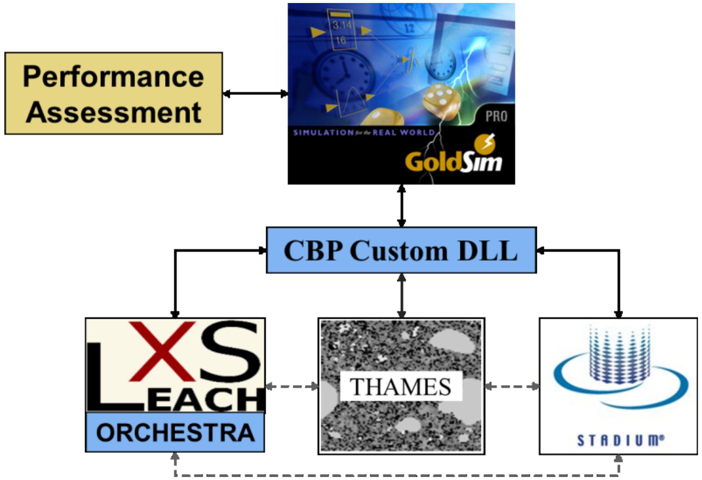
Probabilistic framework

- Integration with GoldSim (www.goldsim.com)

CBP Engagement with PA Process

Conceptual engagement through

- Source-term or boundary condition in near-field
  - for example, radionuclide release from waste form or through barrier
- Material property variations in space and time
  - for example, permeability
- Development of abstracted models

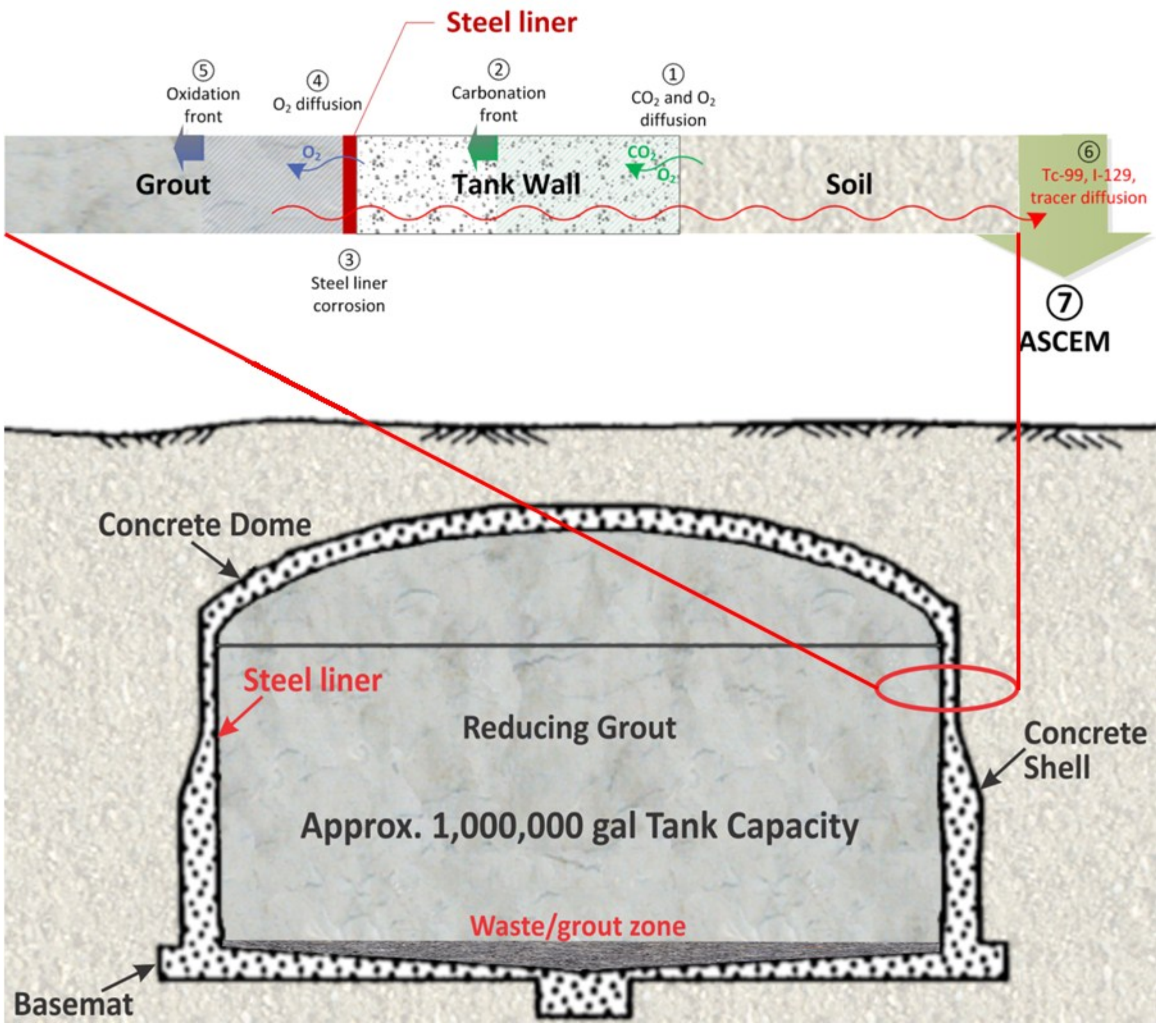


Software engagement through

- GoldSim interface
- Data files (for example, species flux as a function of time)

Example: CBP Source Term

ASCEM-CBP Joint Demonstration



- Relevant for estimating HLW tank system durability and radionuclide retention for
  - Performance assessments (PAs) as part of HLW tank closure
  - Tank integrity for continued use of single shell tanks at Hanford
- Primary phenomena:
  - Concrete carbonation (①&②)
  - Steel liner corrosion (③)
  - Grout oxidation (④&⑤)
  - Contaminant diffusion (⑥)
  - Advective flux of water (⑦)
- ASCEM to simulate far-field to predict nominal flow (⑦)
- CBP to simulate near-field to model tank integrity, leaching, carbonation, corrosion, oxidation, diffusion and radionuclide release (①—⑥)

Example: CBP Source Term

ASCEM-CBP Joint Demonstration

ASCEM far-field flow simulation

Flow field (CBP boundary condition)

CBP near-field simulation

Contaminant leach rate (ASCEM source term)

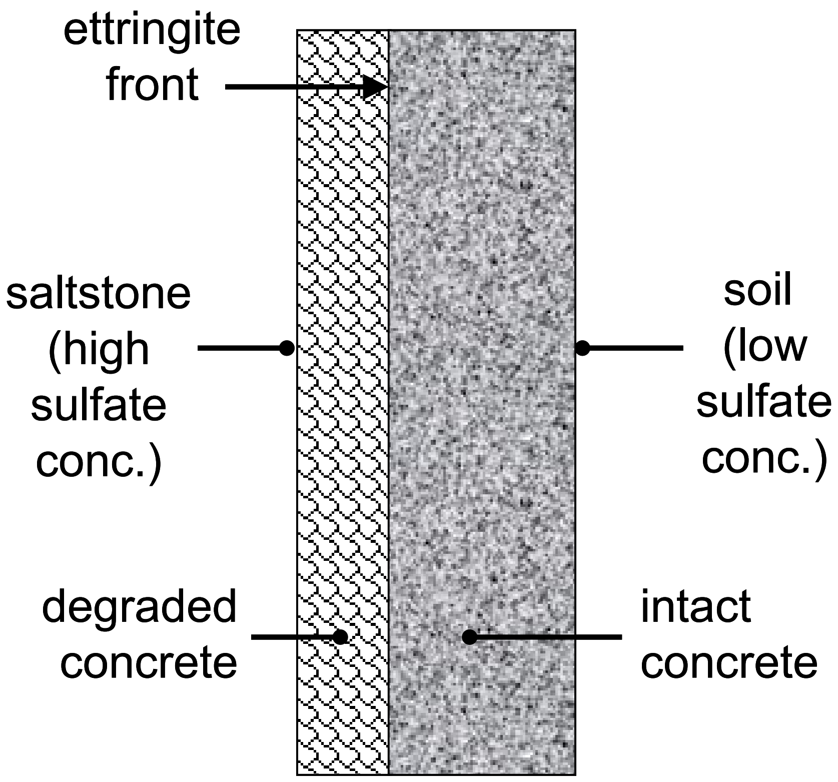
ASCEM far-field transport simulation

Contaminant flux to water table

Example: Effective Property

Approach:

- **STADIUM® code used to predict formation of ettringite (coupled chemistry and transport analysis of major dissolved and solid species)**
- **Simple damage model**
  - Ettringite = physical damage (e.g. cracking, spalling)
  - Transport properties not affected by ettringite front
- **Effective hydraulic properties by averaging**



Example: Effective Property

Abstraction:

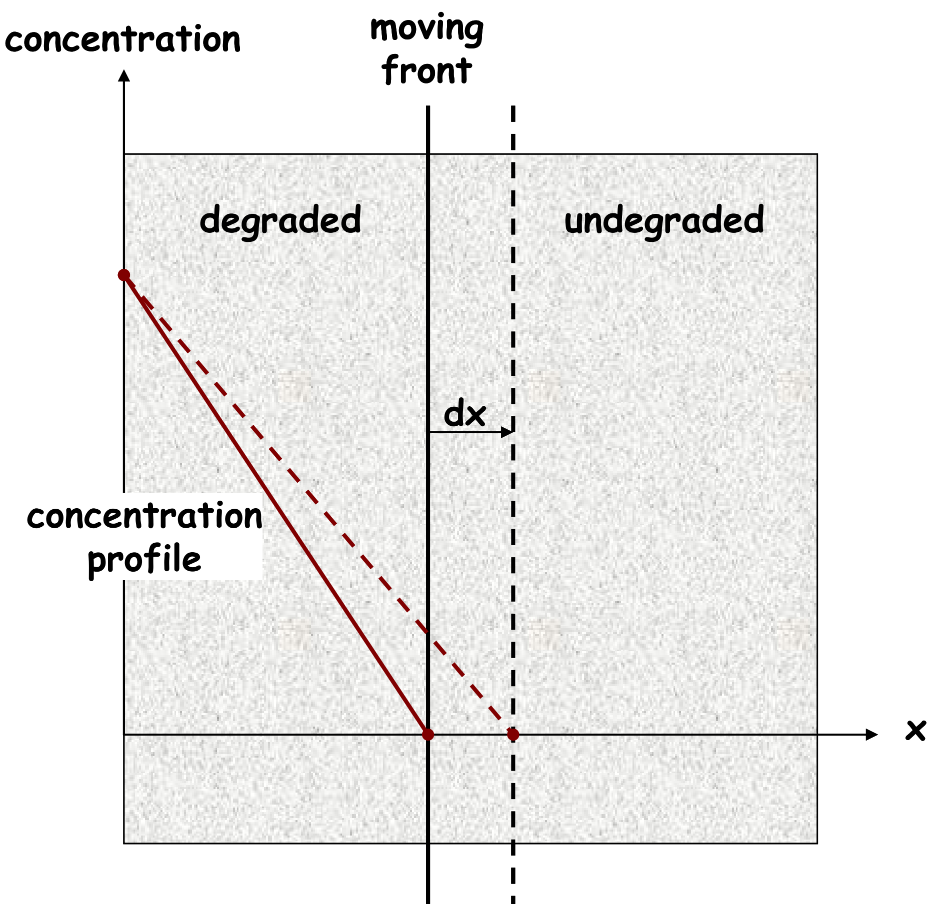
- **Ettringite formation controlled by reaction capacity of concrete, R, and diffusion to front**

$$R\frac{dx}{dt} = \frac{nD_e c}{x}$$

reactant consumption rate | reactant delivery rate

- **Analytic solution for ettringite front**

$$x = \left[\frac{2nD_e ct}{R}\right]^{1/2}$$



Example: Effective Property

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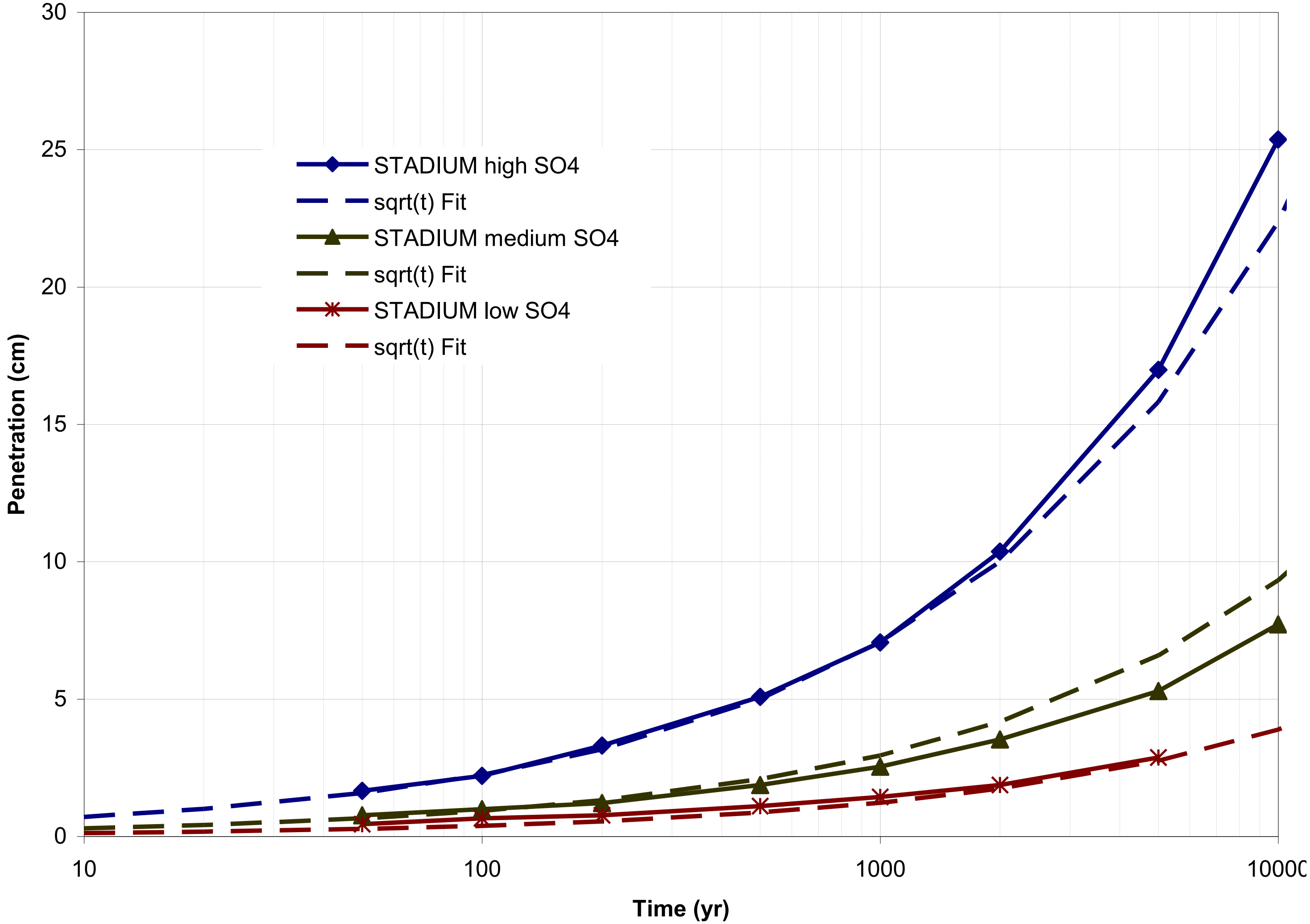
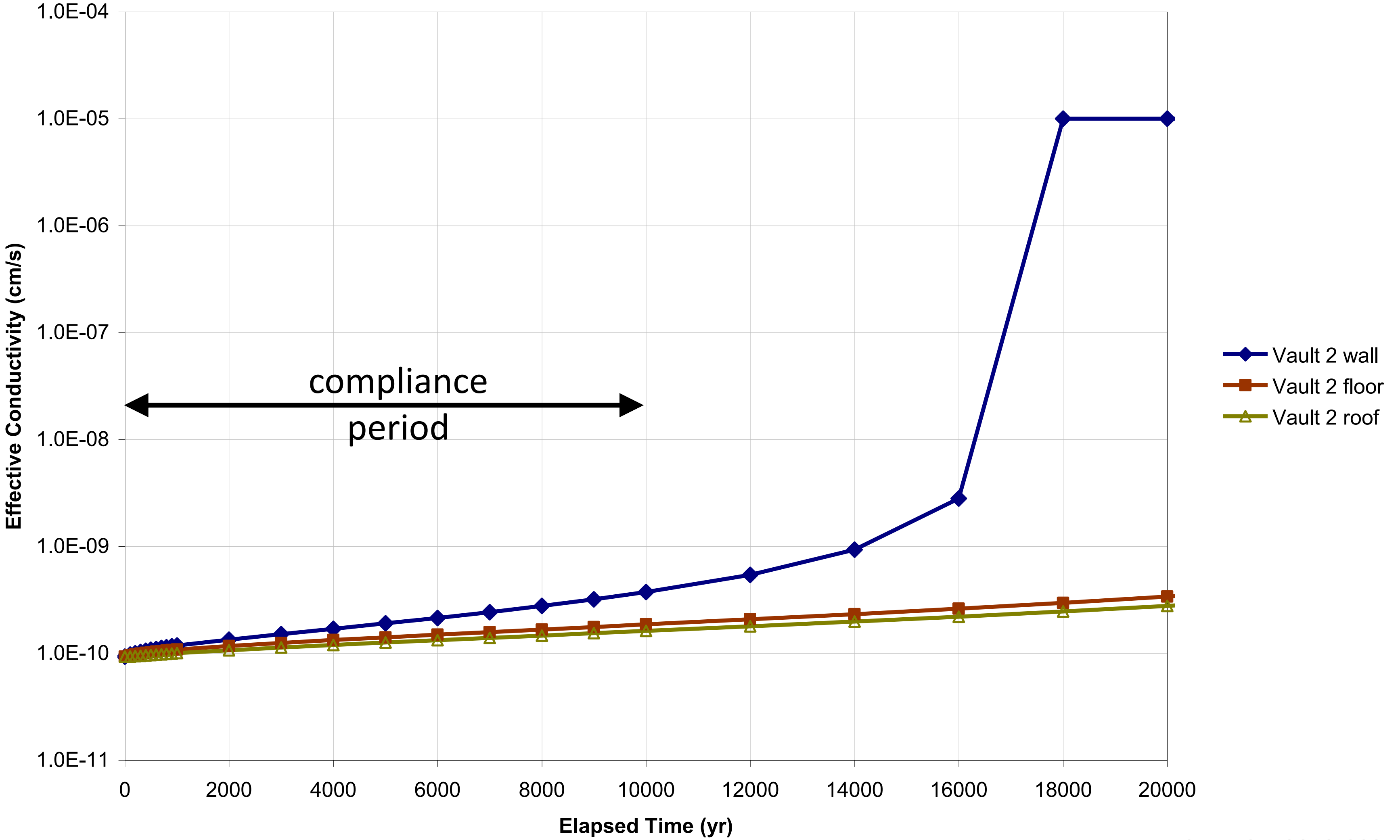
Calibration of reaction capacity to STADIUM®:



Example: Effective Property

Effective Hydraulic Conductivity:



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Summary

- **CBP data and software are designed to address PA challenges arising from**
  - **Long time frames**
  - **Cementitious material degradation**
  - **Uncertainty**
  - **Computing and schedule limitations**
- **CBP software tools can engage the PA process in multiple ways**
  - **Provide higher fidelity models for particular phenomena**
  - **Support model abstraction**
- **CBP tools are 'GoldSim-ready'**